Abstract

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A large scale analysis of information-theoretic network complexity measures using chemical structures

This paper aims to investigate information-theoretic network complexity measures which have already been intensely used in mathematical- and medicinal chemistry including drug design. Numerous such measures have been developed so far but many of them lack a meaningful interpretation, e.g., we want to examine which kind of structural information they detect.

Therefore, our main contribution is to shed light on the relatedness between some selected information measures for graphs by performing a large scale analysis using chemical networks.

Starting from several sets containing real and synthetic chemical structures represented by graphs, we study the relatedness between a classical (partition-based) complexity measure called the topological information content of a graph and some others inferred by a different paradigm leading to partition-independent measures. Moreover, we evaluate the uniqueness of network complexity measures numerically. Generally, a high uniqueness is an important and desirable property when designing novel topological descriptors having the potential to be applied to large chemical databases.